

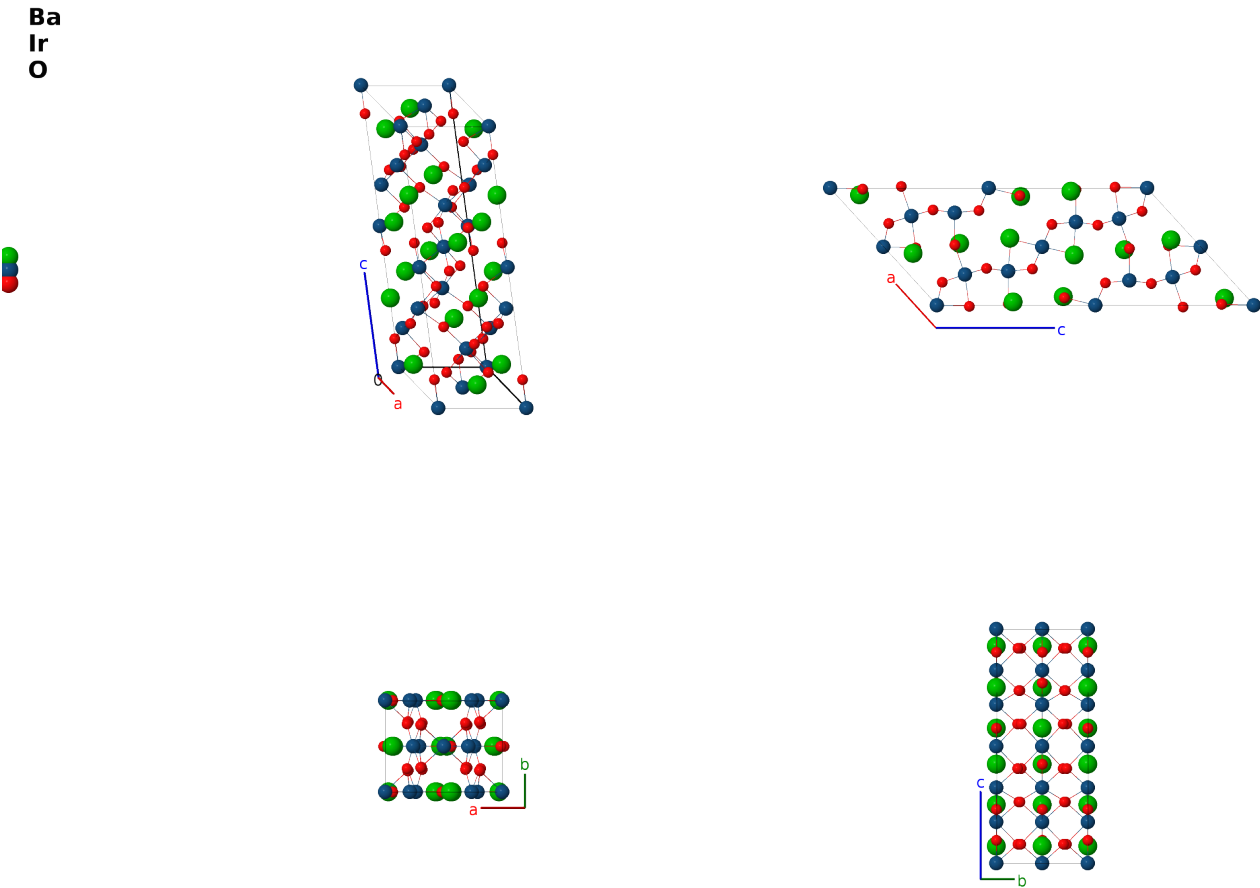
α -BaIrO₃ Perovskite Structure: ABC3_mC60_12_3i_ac2i_3i3j-001

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<https://aflow.org/prototype-encyclopedia/424V>

https://aflow.org/prototype-encyclopedia/ABC3_mC60_12_3i_ac2i_3i3j-001



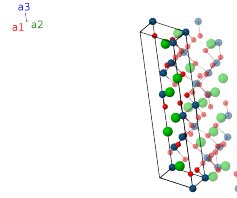
Prototype	BaIrO ₃
AFLOW prototype label	ABC3_mC60_12_3i_ac2i_3i3j-001
ICSD	69720
CCDC	1631570
Pearson symbol	mC60
Space group number	12

Space group symbol	$C2/m$
AFLOW prototype command	afLOW --proto=ABC3_mC60_12_3i_ac2i_3i3j-001 --params= $a, b/a, c/a, \beta, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}$

- BaIrO₃ is a distorted perovskite which has a number of phase transitions with increasing pressure (Cheng, 2009; Cheng, 2013).
- (Cheng, 2009) label the structures by the approximate stacking of the BaO₃ layers.
 - 0-3 GPa: the ground state α -BaIrO₃ “9R” structure, in space group $C2/m$ #12. (this structure)
 - 3-5 GPa: β -BaIrO₃ “5H” structure, also in space group $C2/m$ #12.
 - 5-18 GPa: γ -BaIrO₃, which has the SrIrO₃ “6H” structure.
 - 18-?? GPa: δ -BaIrO₃ is in the tetragonal γ -SrZrO₃ structure.
 - Presumably at some point above 25 GPa the compound transforms into the cubic perovskite ($E2_1$) “3C” structure.
- (Siegrist, 1991) put the second iridium atom at the (2d) Wyckoff position. The AFLOW labeling standard moves this to the (2c) site. This requires a new unit cell: Our $\mathbf{a}_3$ vector is equal to the sum of the (Siegrist, 1991) primitive cell vectors $\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Ir I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2c) Ir II
$\mathbf{B}_3$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Ba I
$\mathbf{B}_4$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Ba I
$\mathbf{B}_5$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Ba II
$\mathbf{B}_6$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Ba II
$\mathbf{B}_7$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Ba III
$\mathbf{B}_8$	=	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Ba III
$\mathbf{B}_9$	=	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Ir III
$\mathbf{B}_{10}$	=	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Ir III
$\mathbf{B}_{11}$	=	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Ir IV
$\mathbf{B}_{12}$	=	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Ir IV
$\mathbf{B}_{13}$	=	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4i) O I
$\mathbf{B}_{14}$	=	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4i) O I

$\mathbf{B}_{15} =$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B}_{16} =$	$-x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B}_{17} =$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B}_{18} =$	$-x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B}_{19} =$	$(x_{11} - y_{11}) \mathbf{a}_1 +$ $(x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
$\mathbf{B}_{20} =$	$-(x_{11} + y_{11}) \mathbf{a}_1 -$ $(x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} -$ $cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
$\mathbf{B}_{21} =$	$-(x_{11} - y_{11}) \mathbf{a}_1 -$ $(x_{11} + y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} -$ $cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
$\mathbf{B}_{22} =$	$(x_{11} + y_{11}) \mathbf{a}_1 +$ $(x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
$\mathbf{B}_{23} =$	$(x_{12} - y_{12}) \mathbf{a}_1 +$ $(x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j)	O V
$\mathbf{B}_{24} =$	$-(x_{12} + y_{12}) \mathbf{a}_1 -$ $(x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j)	O V
$\mathbf{B}_{25} =$	$-(x_{12} - y_{12}) \mathbf{a}_1 -$ $(x_{12} + y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j)	O V
$\mathbf{B}_{26} =$	$(x_{12} + y_{12}) \mathbf{a}_1 +$ $(x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j)	O V
$\mathbf{B}_{27} =$	$(x_{13} - y_{13}) \mathbf{a}_1 +$ $(x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j)	O VI
$\mathbf{B}_{28} =$	$-(x_{13} + y_{13}) \mathbf{a}_1 -$ $(x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} -$ $cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j)	O VI
$\mathbf{B}_{29} =$	$-(x_{13} - y_{13}) \mathbf{a}_1 -$ $(x_{13} + y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} -$ $cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j)	O VI
$\mathbf{B}_{30} =$	$(x_{13} + y_{13}) \mathbf{a}_1 +$ $(x_{13} - y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j)	O VI

References

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